Co-Optimization of Fuels & Engines

Project ID: FT076

Model-based fuel optimization for multi-mode

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June 12, 2019

This presentation does not contain any proprietary, confidential, or otherwise restricted information.

FY19 Vehicle Technologies Office

Annual Merit Review

better fuels | better vehicles | sooner

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

with special thanks to the VTO leadership - David Howell, Gurpreet Singh, Kevin Stork, and Michael Weismiller for their guidance and support

Overview

Timeline

Project start date: FY19
Project end date: FY21*
Percent complete: 17%

Budget

Funding for FY18: $0.3M
- VTO funding: $0.3M
  3 tasks at LLNL, and LBNL
- BETO funding: $0

* *Any proposed future work is subject to change based on funding levels.*

Barriers

Lack of fundamental knowledge about the fuel kinetics impact on engine performance:

- Dilute Gasoline Combustion
- Clean Diesel Combustion
- Low-Temperature & Multi-mode Combustion

Partners

External Advisory Board:

- USCAR, API, Fuels Inst., Truck & Engines Mfg. Assoc., Adv. Biofuels Inst., Advanced Biofuels Association, and Flint Hills Res.
- EPA, CA Air Resources Board
- Dave Foster (U. Wisc.), Ralph Cavalieri (WSU), John Wall (ret. Cummins)

Stakeholders:

85 individuals representing 46 organizations

Universities:

8 FOA awards at 13 institutions (2017 start)

Relevance: Fuel kinetics and simulation tool development address barriers on the 2018 USDRIVE ACEC roadmap

Two critical technologies on the USDRIVE ACEC Tech Team Roadmap* improve with the foundational research in this project (FT076):

1. Dilute Gasoline Combustion

   *"*The three important combustion challenges are combustion robustness (stochastic, cycle-to-cycle combustion variations, partial burns and misfires), operating lean or EGR-diluted over a wide speed and load range, and controlling engine-out emissions of hydrocarbons (HCs) at light loads and nitrogen oxides (NOx) at heavy load."

2. Low Temperature Combustion (including multi-mode) - *strong need for chemical kinetic understanding on modeling*

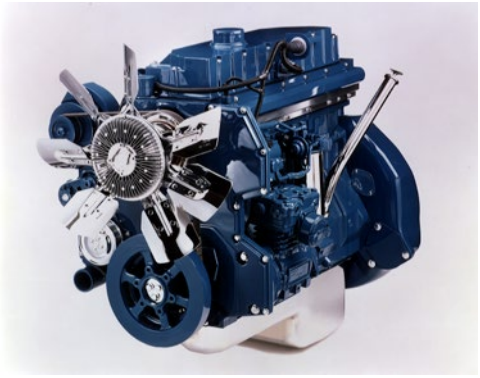
   "[Understand] the impact of likely future fuels on LTC and whether LTC can be more fully enabled by fuel specifications different from gasoline and diesel fuel."

* https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

The governing hypotheses of Co-Optima organize research tasks to address barriers

Co-Optimization Hypothesis:

There are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern internal combustion engines; new fuels are required to maximize efficiency and operability across a wide speed / load range.



Central Fuel Hypothesis

If we identify target values for the critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance.

Co-Optima simultaneously pursues engine and fuel development research within this framework to **increase U.S. competitiveness** by enabling more domestic resources to enter the market, which **creates more jobs for Americans.**

The governing hypotheses provide a common connection from the task outcomes to the program goals

From the hypotheses to the bigger picture:

Co-Optima Goals

Determine key fuel properties that enable improved engine efficiency

Provide key science to enable high efficiency combustion modes

Capitalize on unique properties available from bio-blendstocks

Use stakeholder input to guide analysis

Accelerate market penetration of both engines and fuels.

From the tasks to the hypotheses:

Model-Based Fuel Optimization (FT076)

Predict blending behavior for High Performance Fuels and petroleum components

Predict fuel kinetic property impact on engine efficiency and Co-Optimization Hypothesis

Create a virtual fuel designer to test the Central Fuel Hypothesis

Accelerate the time to solution for all fuel kinetics based analyses

Optimize fuel composition for multi-mode performance (see Sjoberg's AMR talk FT070)

Milestones

Date	Description of Milestone or Go/No-Go Decision	Status	Lab
Sep 2018	G.4: Measure the uncertainty quantification performance using a hierarchy of kinetic-based engine models at varying levels of chemical and fluid dynamic fidelity.	done	LLNL
Dec 2018	G.4.LBNL(b): Develop a bi-level optimization approach that optimizes fuel properties at the upper level and engine configurations at the lower level to achieve optimized fuel-engine configurations.	done	LBNL
Mar 2019	G.1.1: Report on the accuracy improvements to the octane model prediction performance using simulated engine operation as input features.	done	LLNL
Jun 2019	G.5.3: Report on the fuel blends found to have the most (and least) high efficiency operating range for a fixed RON and S based on the supercomputer search, with testable blend recommendations for engine validation.	on-track *see FT070*	LLNL
Jun 2019	G.4.LBNL(a): Validate a data-driven statistical model (e.g. Gaussian Process Regression) that can be trained with experimental and simulated fuel-engine data to propose new test conditions that reduce uncertainty between the bookends of the p-T-* space.	on-track *see FT070*	LBNL
Sep 2019	G.4.LBNL(a): Scenario Co-optimizer: Implementation of surrogate models and development of new sampling strategy for globally robust predictions	on-track	LBNL

Task budgets - planned FY19 costs

Task	Description	FY19 costs	Lab
G.1.1	[McNenly] Virtual properties, reduced mechanism, blending of kinetics properties, and modeling of Fuel Properties	$200K	LLNL
G.1.2	[McNenly] Accelerating Co-Optima applications with Zero-RK	$50K	LLNL
G.1.8	[Grout] Understanding how kinetics limit multi-mode performance	zero	NREL
G.4	[J. Mueller] Surrogate model development	$75K	LBNL
G.4	[Grout] Data driven interpretation and experimental design	zero	NREL

Approach - Accelerate hypothesis testing using accurate fuel chemistry models for broad blend explorations

Step 1. Define a performance metric (Q) that can be simulated with chemical kinetics (in collaboration with engine experimentalists):

$$Q\begin{pmatrix} RPM \\ CR \\ \mathrm{C_2H_5OH} \\ n\text{-}\mathrm{C_7H_{16}} \\ i\text{-}\mathrm{C_8H_{18}} \\ \cdots \end{pmatrix}$$

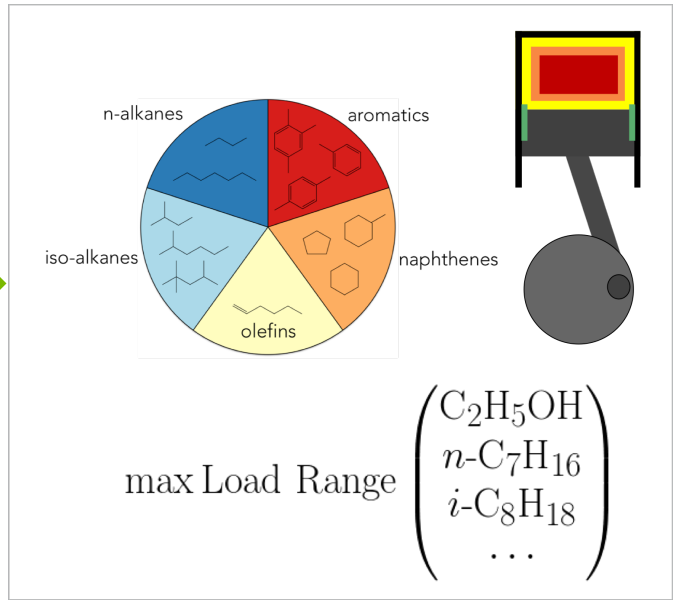
Current and previous research:

- Maximize phi-sensitivity and octane sensitivity at RON > 95 (2017 AMR).
- Maximize each PIONA class at a fixed RON and MON to test the Central Fuel Hypothesis for BOB blending (2018 AMR).
- Maximize the load range and number of feasible operating conditions for DISI multi-mode performance (2019 AMR).

Approach - Accelerate hypothesis testing using accurate fuel chemistry models for broad blend explorations

Step 2. Create a computationally efficient simulation of the metric capable of using the highest fidelity Co-Optima mechanism.

$$Q \begin{pmatrix} RPM \\ CR \\ \mathrm{C_2H_5OH} \\ n\text{-}\mathrm{C_7H_{16}} \\ i\text{-}\mathrm{C_8H_{18}} \\ \cdots \end{pmatrix}$$



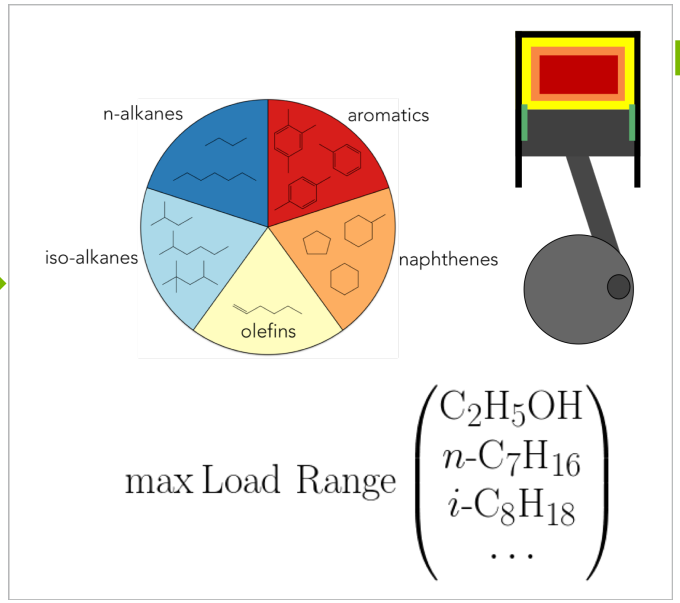
Available and future kinetic-based engine and fuel property models:

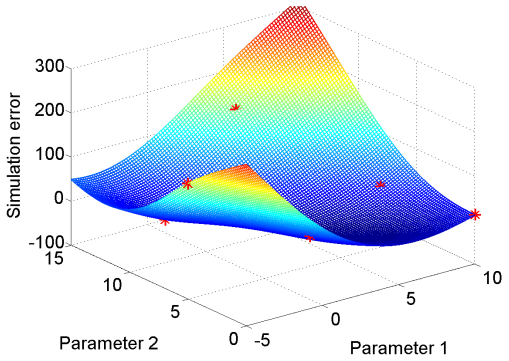
- Homogenous reactor, including variable volume or variable pressure trained by GT-Power
- Multi-zone auto-ignition model
- Laminar flame speed (pre-mixed and diffusion flames)
- Neural network octane models
- Multi-zone engine model with flame propagation (proposed FY20)
- Stochastic reactor model with CFD-trained mixing models for stratified control (proposed FY20)

Approach - Accelerate hypothesis testing using accurate fuel chemistry models for broad blend explorations

Step 2b. [if needed] Create a data-driven surrogate model using the simulation results to explore a much larger range of compositions and conditions.

$$Q \begin{pmatrix} RPM \\ CR \\ \mathrm{C_2H_5OH} \\ n\text{-}\mathrm{C_7H_{16}} \\ i\text{-}\mathrm{C_8H_{18}} \\ \cdots \end{pmatrix}$$

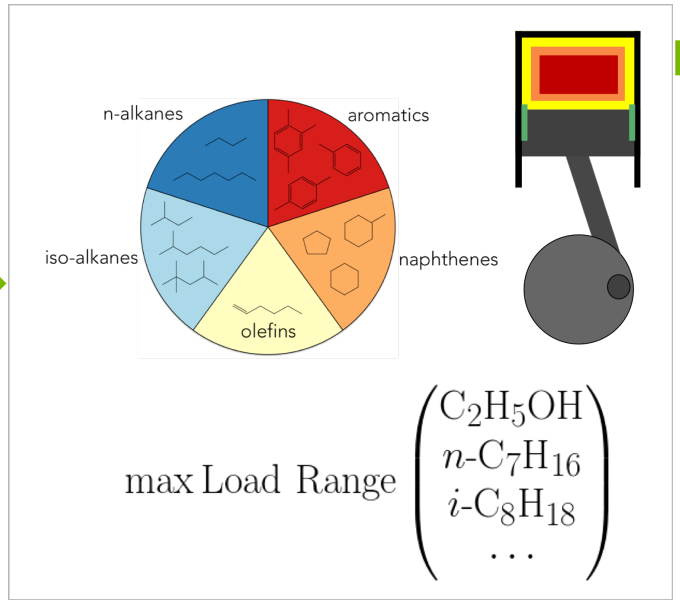


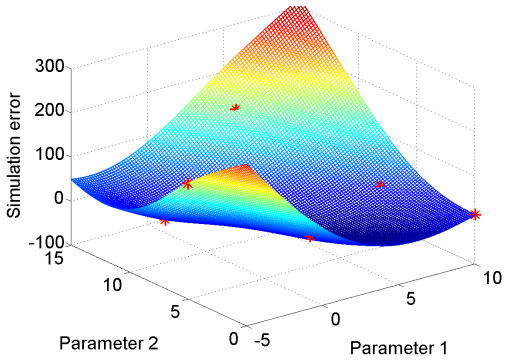


Approach - Accelerate hypothesis testing using accurate fuel chemistry models for broad blend explorations

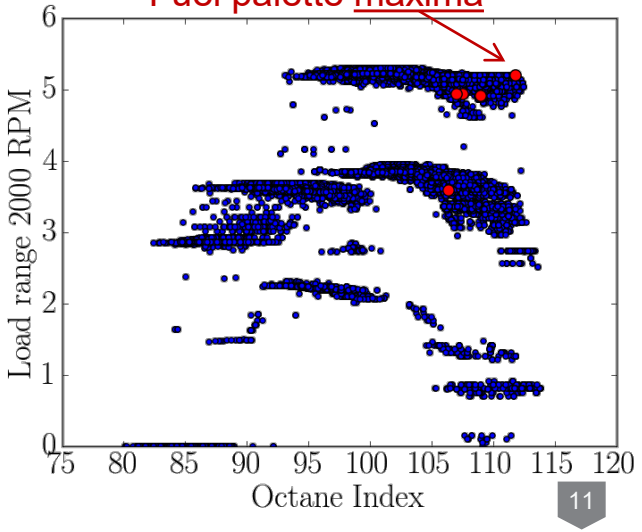
Step 3. Search for compositions and engine conditions that maximize the desired performance metric predicted in the model.

$$Q \begin{pmatrix} RPM \\ CR \\ \mathrm{C_2H_5OH} \\ n\text{-}\mathrm{C_7H_{16}} \\ i\text{-}\mathrm{C_8H_{18}} \\ \cdots \end{pmatrix}$$





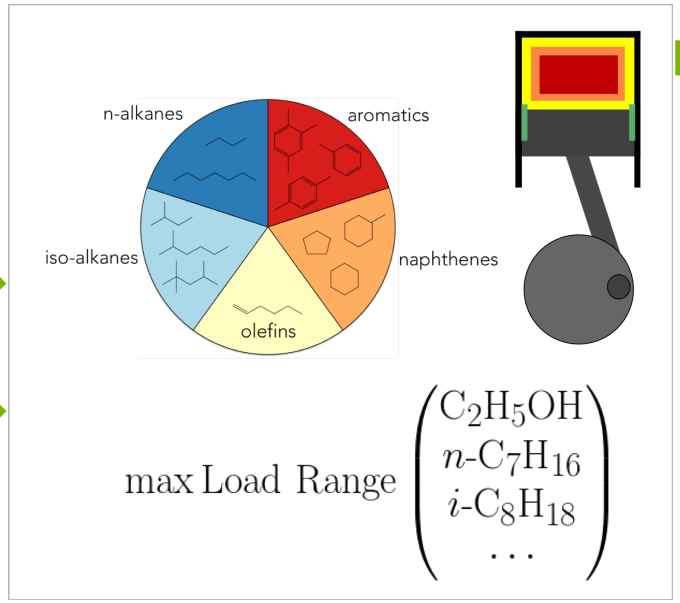
Fuel palette maxima

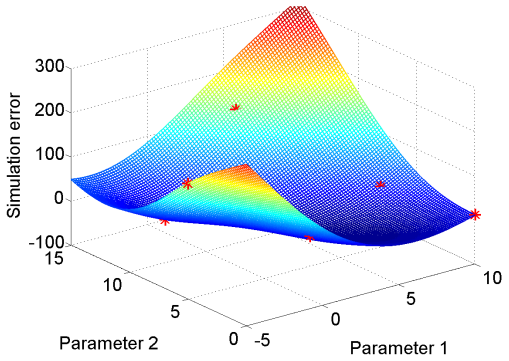


Approach - Accelerate hypothesis testing using accurate fuel chemistry models for broad blend explorations

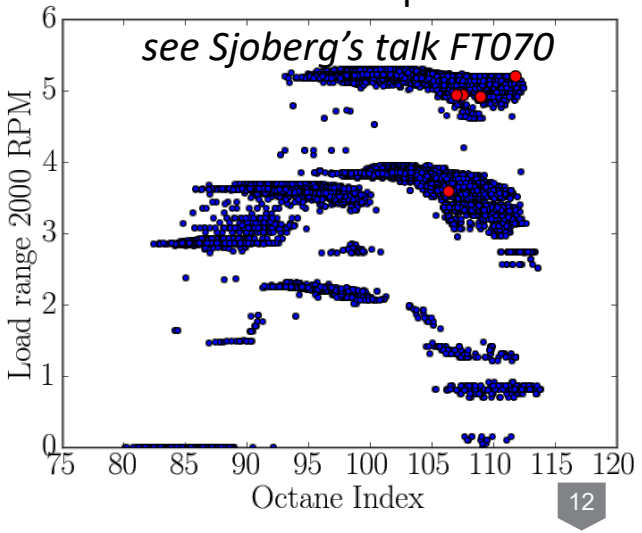
Step 4. Validate the predicted fuel impact on engine performance in a physical experiment.

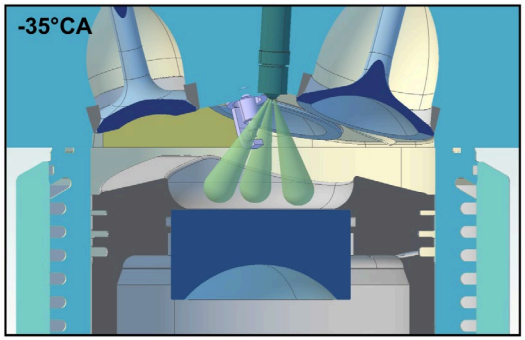
$$Q \begin{pmatrix} RPM \\ CR \\ \mathrm{C_2H_5OH} \\ n\text{-}\mathrm{C_7H_{16}} \\ i\text{-}\mathrm{C_8H_{18}} \\ \cdots \end{pmatrix}$$

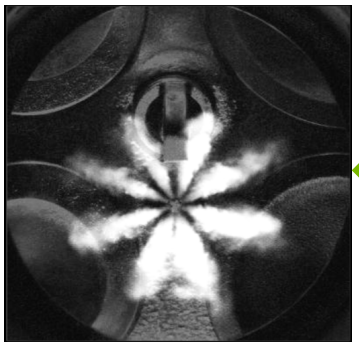




Multi-mode fuel optimization



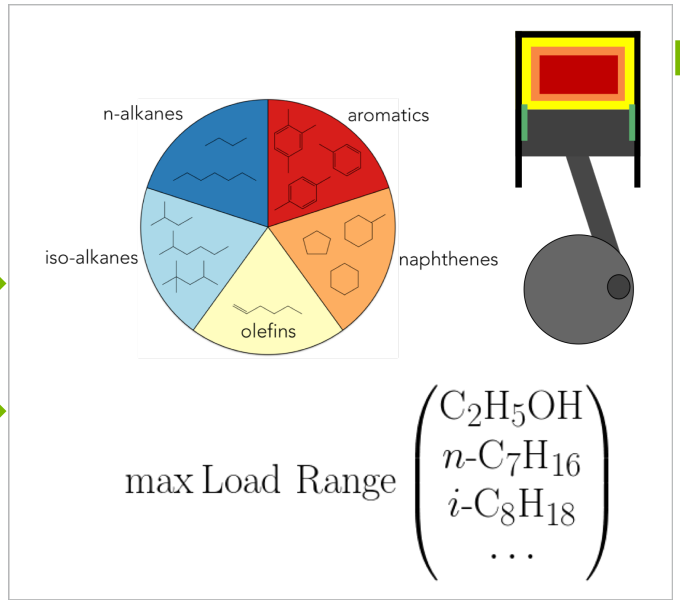


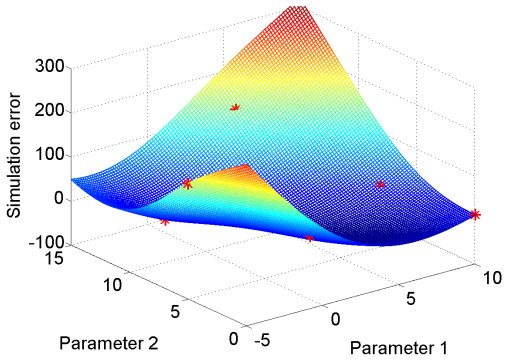


Approach - Accelerate hypothesis testing using accurate fuel chemistry models for broad blend explorations

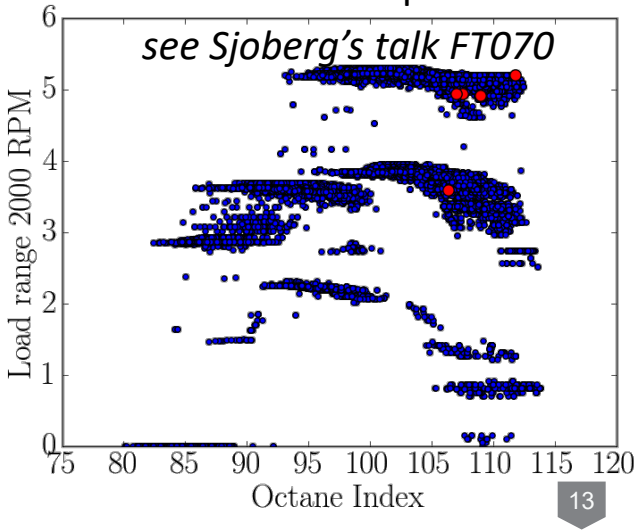
Step 5. Depending on the outcome of Step 4, improve the kinetics, the engine model, or the operating conditions and repeat...

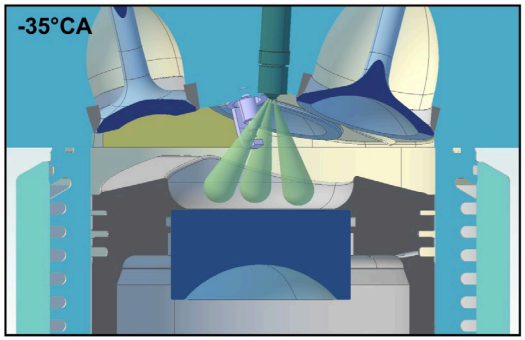
$$Q \begin{pmatrix} RPM \\ CR \\ \mathrm{C_2H_5OH} \\ n\text{-}\mathrm{C_7H_{16}} \\ i\text{-}\mathrm{C_8H_{18}} \\ \cdots \end{pmatrix}$$

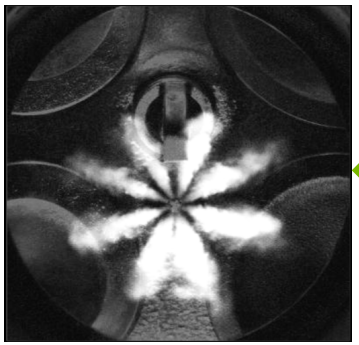




Multi-mode fuel optimization







The potential for co-optimization can be enhanced through careful exploitation of non-linear blending behavior

To study fuel property tradeoffs in multi-mode applications, accurate models for the octane numbers are needed to ensure high-load engine performance:

1. Linear blending models can not capture synergistic/antagonistic effects common with bio-derived blendstocks.
2. Correlations based on zero-dimensional ignition simulations provide better estimates but fail in some cases (max abs. error ~10 ON, r.m.s. error ~2 ON).
3. Neural Network (NN) model using ignition simulations and other readily available fuel mixture properties were presented in FY18 with lower errors.

1. $$\mathrm{RON}_{pred} = \sum_{i=0}^{nsp} x_i \mathrm{RON}_{i,measured}$$

2. $$\mathrm{RON}_{pred} = f(\tau_{ign})$$

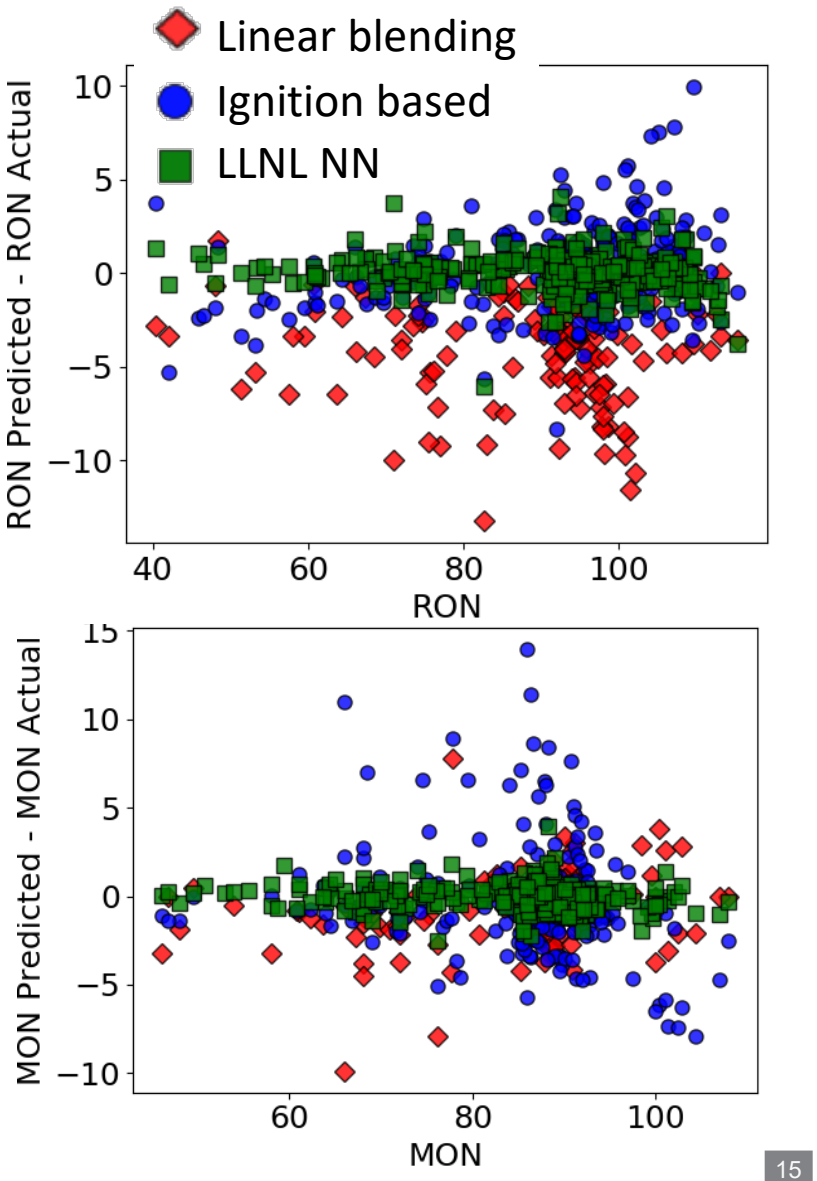
3. $$\mathrm{RON}_{pred} = f(\tau_{ign}, \mathrm{HOV}, \mathrm{structure}, \ldots)$$

Surrogate fuel blends can be any combination of the 31 hydrocarbon and 25 high performance blendstocks from the Co-Optima gasoline surrogate.

[2018 AMR] Nonlinear octane blending model predicts RON and MON with r.m.s. error less than 2.3

LLNL Neural Network Octane Model (2018 version):

- New approach improved prediction of RON and MON
- Easy to build virtual surrogate fuels to test blending effects
- Fast CPU run-time enables broad fuel blend explorations
- Room for improvement:
  - Outliers still remain and testing on new data was not completely satisfactory
  - Published model (KAUST) claims accuracy better than measurement repeatability



Nonlinear octane blending model predicts RON with r.m.s. error of 0.8 on ten previously untested blends

NN octane model improved (FY19 Q2 Milestone)*

- New CFR Engine Data
  - References (~30 total, 15 prev.)
  - Measurements (486 from 359)
- Data cleanup and feature design
- Better training process
- New molecular structure information

Comparison with KAUST NN model:

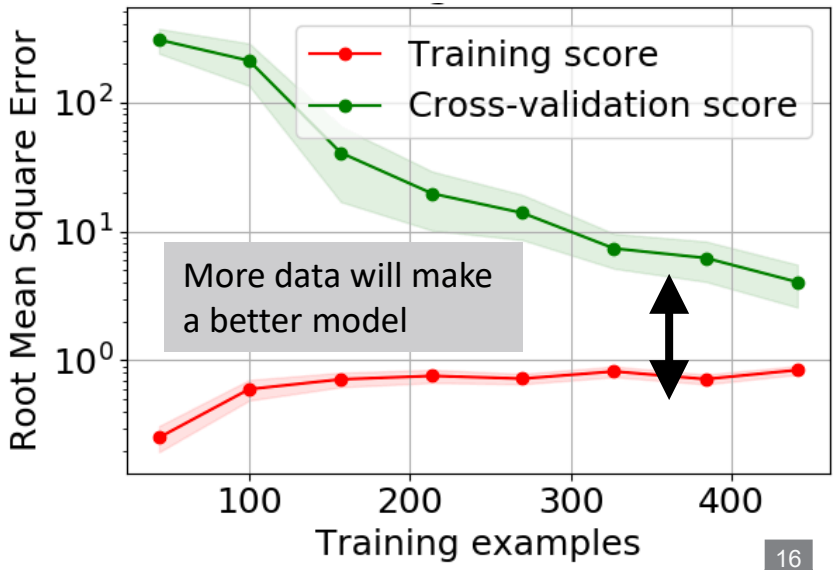
- Designed for surrogates and refinery streams (based on NMR data)
- Ethanol only oxygenated species included in model

KAUST NN - doi:10.1021/acs.energyfuels.8b00556

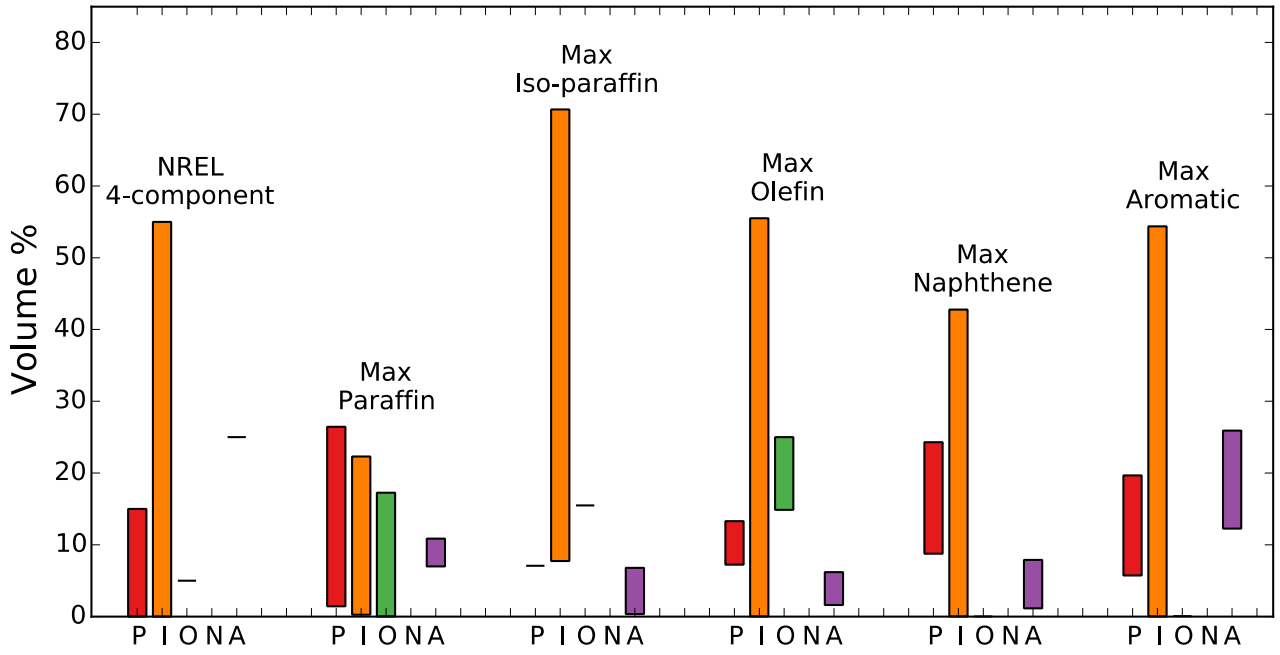
Performance validated on ten previously untested 9-component BOB surrogates:

Model	RON r.m.s. error	MON r.m.s. error
KAUST	2.3	4.8
LLNL FY18	2.2	2.3
*LLNL FY19	0.8	1.4

RON NN Training Curve



[2018 AMR] Created five virtual BOBs with a model RON of 90.3 +/- 0.1 and model MON of 84.7 +/- 0.1



(P) araffins
- n-pentane
- n-heptane

(I) so-paraffins
- iso-pentane
- iso-octane

(O) lefins
- 1-hexene
- diisobutylene

(N) aphthenes
- cyclopentane

(A) romatics
- toluene
- 1,2,4-trimethylbenzene

NREL 4-component BOB

55% iso-octane (by vol.)
25% toluene
15% n-heptane
5% 1-hexene

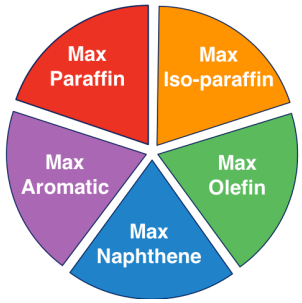
ASTM ratings*:

RON	90.3
MON	84.7

* McCormick, R., Fioroni, G., Fouts, L., Christensen, E. et al., "Selection Criteria and Screening of Potential Biomass-Derived Streams as Fuel Blendstocks for Advanced Spark-Ignition Engines," *SAE Int. J. Fuels Lubr.* 10(2):442-460, 2017, https://doi.org/10.4271/2017-01-0868. (SAE Paper No. 2017-01-0868)

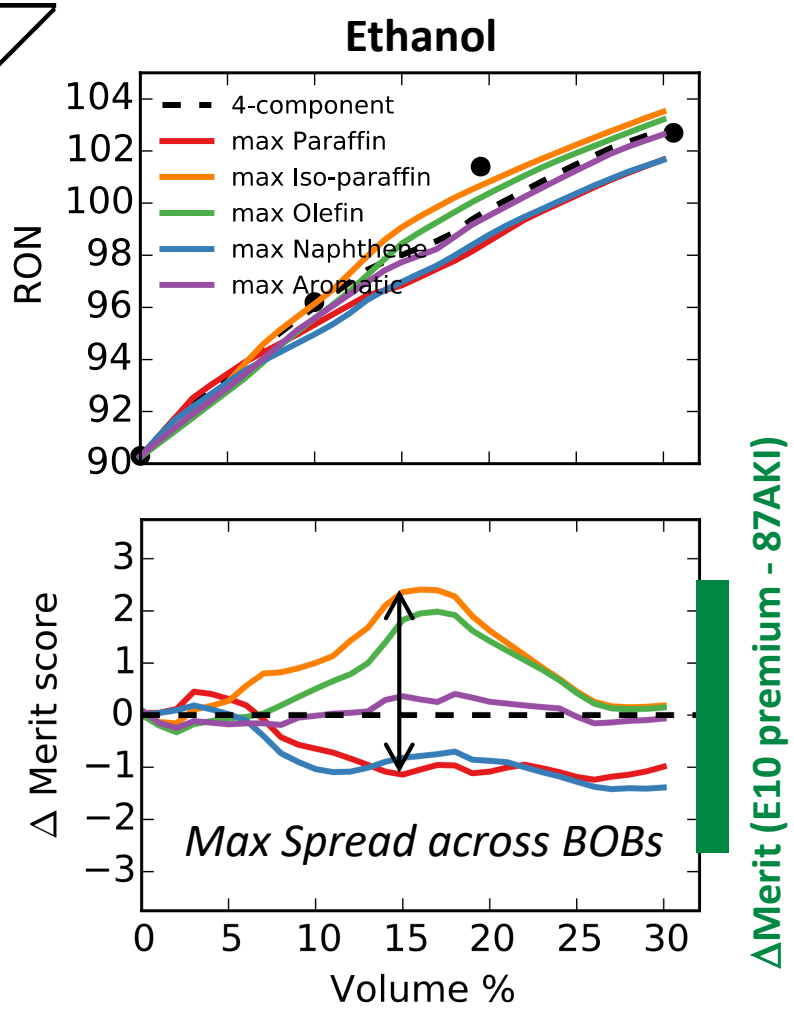
[2018 AMR] Model-based variation in BOB merit scores is ~60% of the net gain switching from 87 AKI to E10 premium

Blendstocks	Merit Score Error	RON Spread	Most Antagonistic	Most Synergistic	Sensitivity Spread	Most Antagonistic	Most Synergistic	Merit Score Spread	Most Antagonistic	Most Synergistic
2-butanol	1.1	1.9			3.1			3.6		
2-methyl-1-propanol	1.8	2.6			2.4			3.5		
ethanol	1.8	2.4			2.7			3.5		
diisobutylene mix	2.1	2.7			1.0			2.4		
methanol	1.6	2.3			3.0			3.5		
furan mix	1.2	2.3			3.5			3.4		
methoxybenzene	4.4	2.9			2.4			2.9		
cyclopentanone	2.3	1.6			3.1			2.5		
2-pentanone	2.9	3.2			3.8			4.4		
methylacetate	2.6	3.1			2.9			4.2		
3-pentanone	1.5	2.9			3.0			4.1		
2-propanol	0.6	2.7			2.8			3.7		
ethylacetate	3.0	2.9			2.8			3.4		
1-propanol	1.3	2.8			2.1			3.3		
2-methyl-1-butanol	1.1	1.8			1.2			1.7		
1-butanol	1.0	1.5			1.9			1.7		
3-methyl-1-butanol	0.5	1.5			1.0			1.4		



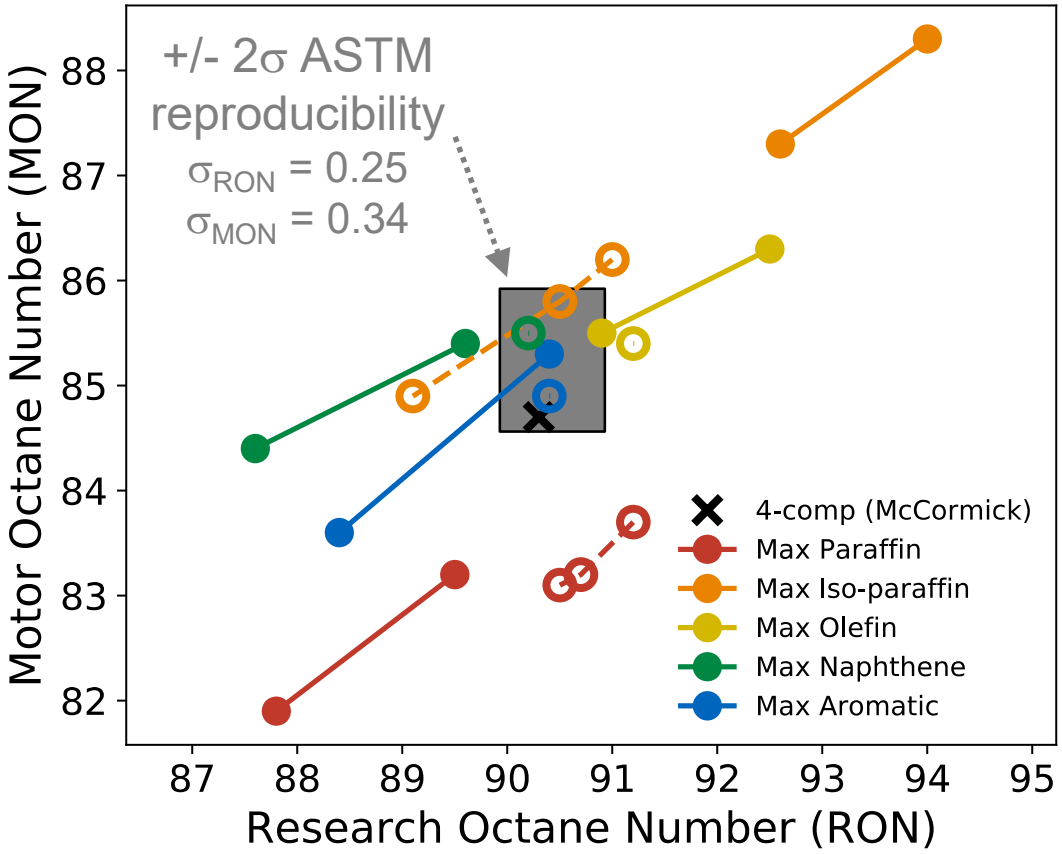
NREL 4-component BOB

55% iso-octane (by vol.)
25% toluene
15% n-heptane
5% 1-hexene



The octane model performance for BOB optimization to be validated with 120 new RON and MON measurements

Phase 1a (filled) and Phase 1b (open) BOB design



Phase 1a (filled) used high purity 2,4,4-trimethyl-1-pentene

Phase 1b (open) used lower cost 3:1 mix of diisobutylene isomers

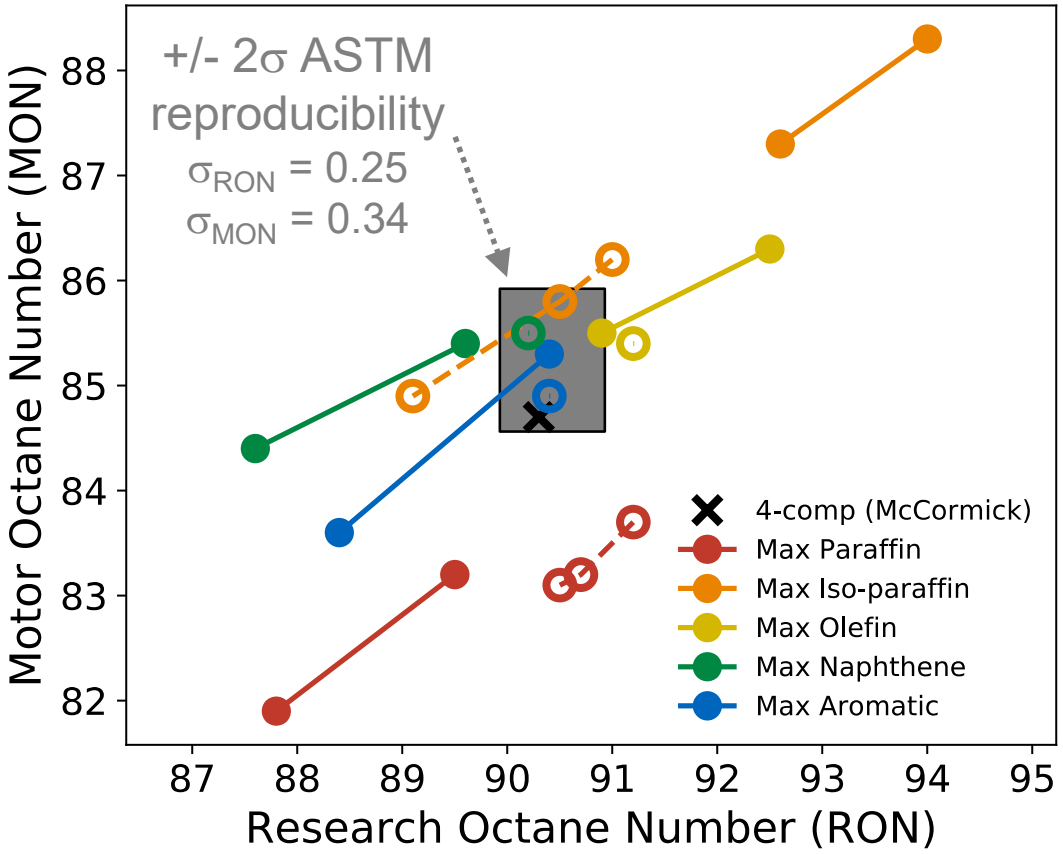
Validation Approach

Phase 1:

1. The five max-PIONA class BOBs are created using the model derived recipes for Phase 1a.
2. A second set of five are also created with a model RON two ON lower for Phase 1a.
3. Three BOBs validated in Phase 1a for HPF blending using standard ASTM tests.
4. The validated max iso-paraffin was found by further lowering RON in Phase 1b.
5. The max paraffin blend will be finalized in Phase 1c (FY19Q3).

The octane model performance for BOB optimization to be validated with 120 new RON and MON measurements

Phase 1a (filled) and Phase 1b (open) BOB design



Phase 1a (filled) used high purity 2,4,4-trimethyl-1-pentene

Phase 1b (open) used lower cost 3:1 mix of diisobutylene isomers

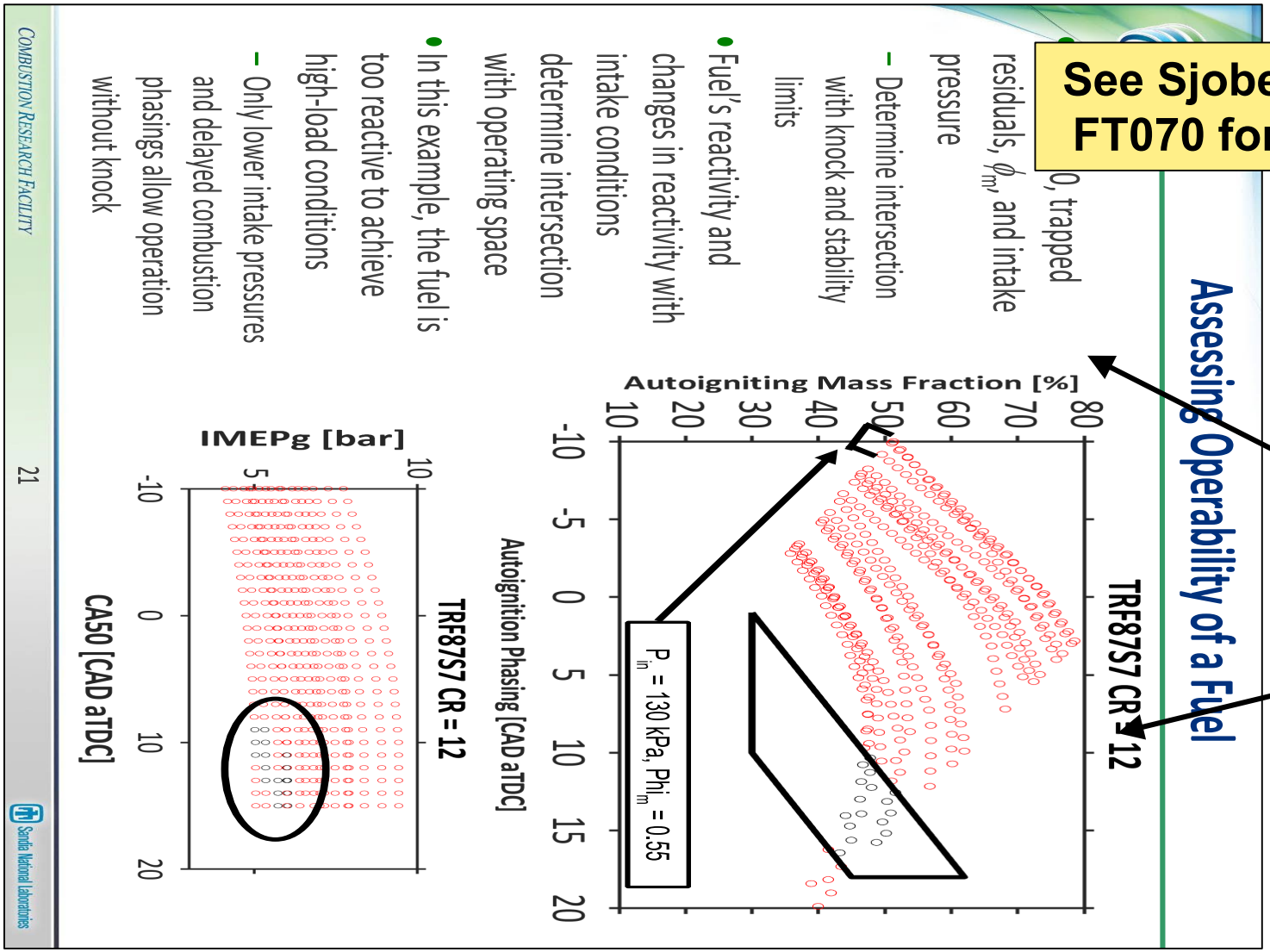
Validation Approach

Phase 2:

6. Phase 2 blends six HPF blendstocks at 10, 20 and 30% into the five max-PIONA BOBs to quantify merit score variation with composition:
   a. ethanol
   b. iso-butanol
   c. 3-pentanone
   d. methylacetate
   e. 2-methylfuran
   f. diisobutylene

Phase 2 - 60% complete
(Max Olefin, Max Naphthene and Max Aromatic tested)

Kinetic model-based metric for optimizing spark-assisted compression ignition developed at SNL



See Sjoberg's AMR talk FT070 for more details

Two Objectives

Maximize:

1. # of Operable Conditions (Robustness)
2. Operable IMEP Load Range

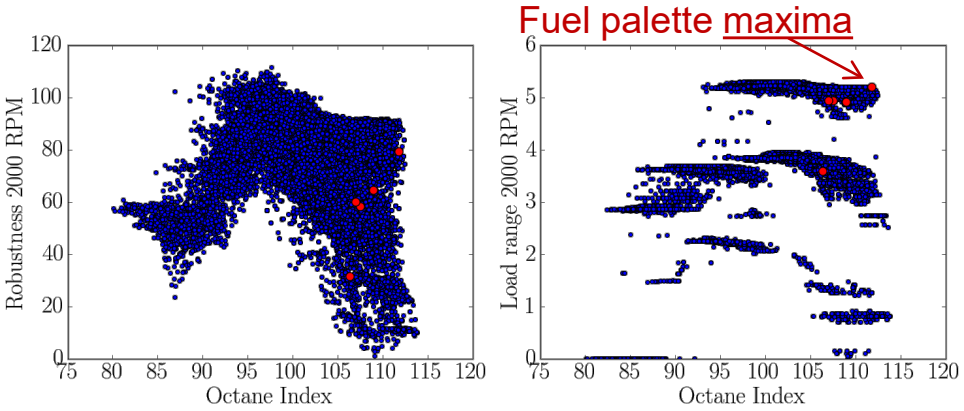
D. Vuilleumier, N. Kim, and M. Sjoberg, "Fuel effects on mixed-mode combustion in a DISI engine," AEC Program Review Meeting, Knoxville, TN, Jan. 2019.

LLNL's advanced chemistry solver Zero-RK is used to speedup the multi-mode model by more than a factor of 10

Features of the multi-mode model developed for DISI by Vuilleumier, Kim and Sjoberg (SNL):

- GT-power engine model solves the pressure time history for each condition.
- Pressure history serves as input to 0D variable pressure reactor.
- 0D model computes the autoignition phasing.
- Experimentally determined operability envelop relates auto-ignition phasing simulations to the two performance objectives (robustness & IMEP load range).
- Each blue dot represents one fuel composition, which is the result of 864 auto-ignition phasing calculation.
- Wide range of engine conditions covered: spark timing, engine speed, intake pressure, compression ratio, BDC temperature, equivalence ratio.

Simulated Performance Objectives for 50,000 Blends (1 of 3 speeds shown)

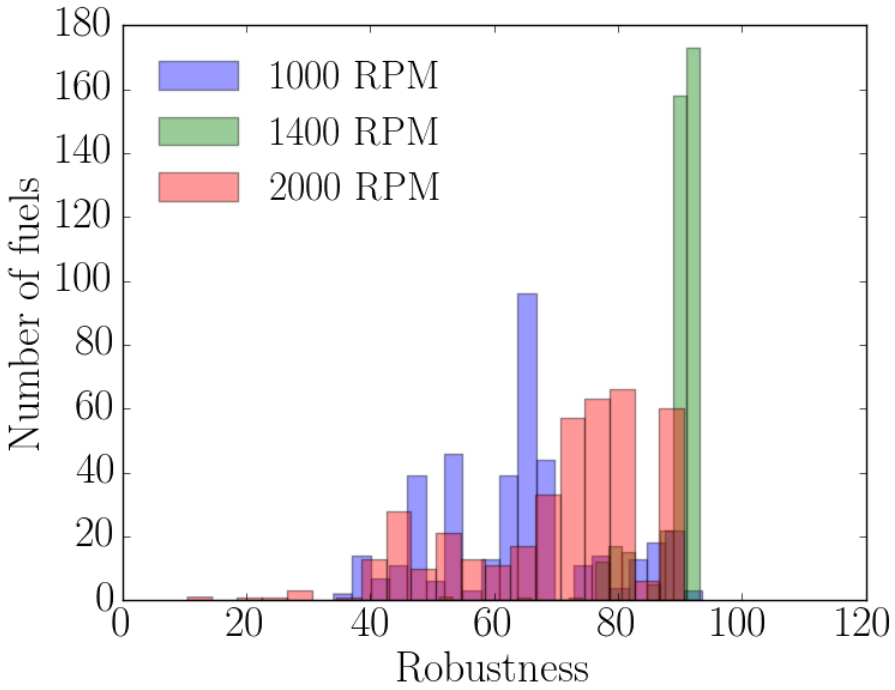


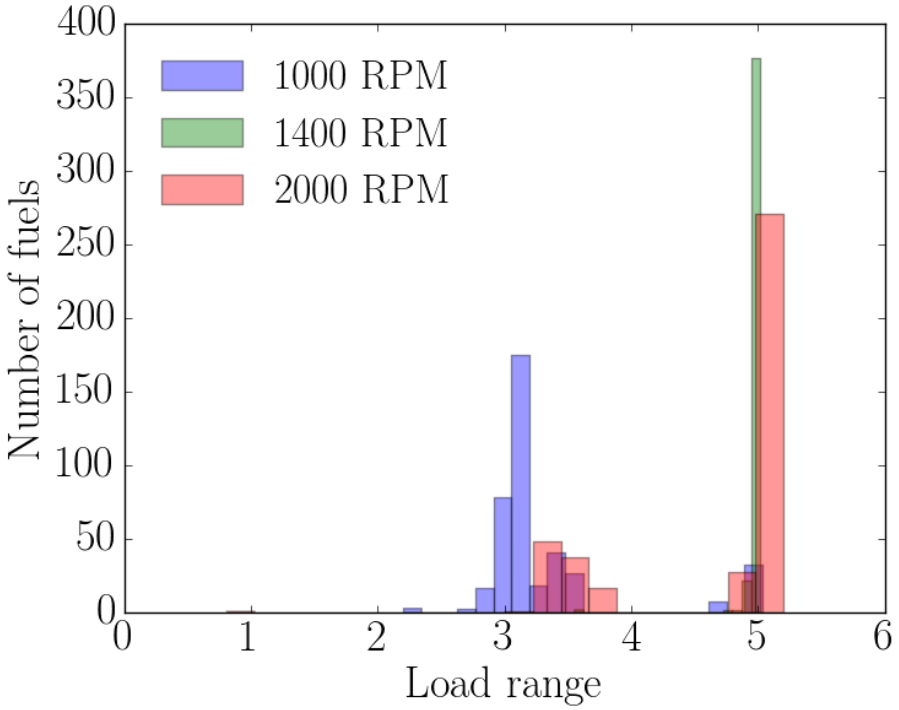
LLNL Simulation Toolkit Enhancements (Lapointe):

- Zero-RK delivers 10-40x speedup over previous Chemkin Pro model (serial).
- Further speedup achieved by parallelizing over the engine operating conditions.
- Python wrapper created to take advantage of large suite of open source optimization tools.

Initial search of 50,000 fuel blends shows large spread in performance even at similar RON and MON

All fuel blends in the histogram have a similar octane rating - RON 97 & MON 85





- RON and Octane Index show some correlation to the multi-mode engine performance (see FT070), but very noisy.
- Without new fuel property/performance metrics, Central Fuel Hypothesis does not appear to hold in the multi-mode simulations.

Next Steps:

- Find compositions that yield a max and min robustness and load range for the same octane rating.
- Validate the model-based search results in multi-mode engine tests at SNL.

Response to reviewers

1. "One criticism the reviewer had about the work is the lack of consideration of turbulence in the evaluation of ignition delay times." "The reviewer urged thinking about including the effects of turbulence chemistry."

   Response: An accelerated stochastic reactor engine model is planned for FY20. The turbulent mixing rates for mass, species and heat will be trained from detailed CFD simulation performed at ANL. The model will have a low enough computational cost to conduct fuel blend optimization studies to improve mixed-mode controllability in regimes where the ignition kinetics and turbulent mixing have similar timescales. Turbulent chemistry models for use in high-fidelity CFD simulations are in the scope of the Combustion Consortium (formerly the core research program of the VTO Advanced Combustion Systems sub-program).

2. "To make the knowledge more transferable to industry, mechanism reduction is critical and should be addressed."

   Response: The Zero-RK fast chemistry solver was used to accelerate the mechanism reduction tools of Prof. Niemeyer (Oregon St. Univ.) and has been provided to chemical kinetics team at LLNL to make reduced versions of real fuel surrogates more widely available outside Co-Optima.

3. "To search for the right fuel chemistry for the multimode ACI/SI operation, the reviewer commented that the project team needs to present a merit function to rank different combinations."

   Response: This has been our long-term goal since the start of Co-Optima. Please check out the promising results for the metric proposed by Vuilleumier, Kim and Sjoberg for DISI multi-mode operation (Sjoberg's AMR talk FT070, and Vuilleumier's AEC Program Review Talk, Jan. 2019).

Collaboration and coordination

Within the Co-Optima program

- Created virtual fuel models with matched octane ratings for the ANL CFD simulations.
- Isolated molecular class impacts on synergistic blending with Sutton (LANL) for the High Performance Fuels team.
- Developed a data driven statistical modeling for the boosted SI experiments by Szybist (ORNL).
- Optimized BOB composition to maximize synergistic and antagonistic blending for six bio-derived fuels with McCormick, Fioroni and Fouts (NREL).
- Searched +50,000 fuel compositions for blends that maximize multi-mode load range for Sjoberg and Vuilleumier (SNL).
- Recent FOA awards to 8 projects at 13 universities includes two groups with which LLNL mentors or collaborates:
  - Prof. Xuan's group, Penn. St. Univ: model soot production using the Co-Optima HPFs fuel kinetic models for the YSI experiments - Lapointe (LLNL) created a high performance diffusion flame solver
  - Prof. Schoegl's group, Louisiana St. Univ.: micro-scale flow reactor to estimate fuel properties with microliters sample volumes

Remaining challenges and barriers

- Increasing the accuracy of real fuel models to co-optimize fuels & engines
- Validating chemical kinetic models over wider pressure ranges, equivalence ratios, EGR dilution levels, and blending – *need lots of data*
- Producing experimental kinetic data for a large number of blendstocks and blending levels in a short time frame with very small sample volumes – *need small volume, high throughput ignition testing methods*
- Identifying the dependency between critical chemical pathways and functional groups and engine performance
- Searching for optimal fuel surrogate blends for expected engine performance, including multi-mode combustion strategies
- Establishing error bars on kinetic simulation results such that fuel-engine comparisons have a confidence percentage.
- Creating a framework to fairly compare the benefits of different mixed-mode strategies and fuel combinations.

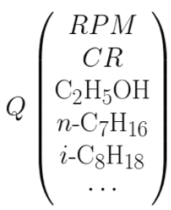
Proposed future work*

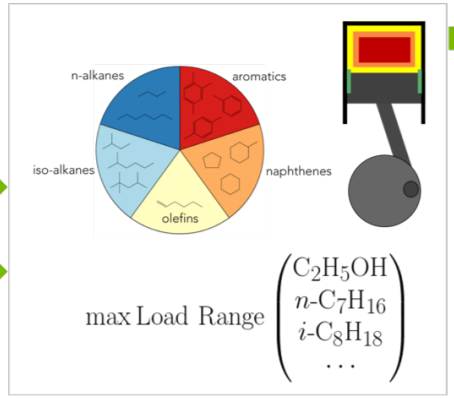
LLNL
- Continue research to identify the chemical kinetic sources for phi-sensitivity and synergistic octane blending.
- Continue search for co-optimized fuel blends and engine parameters that maximize speed-load range for acceptable operation of the high-efficiency, low power mode, based on the multi-mode platform at SNL (Sjoberg).
- Find Co-Optimized fuel blends and engine parameters that maximize lean/dilute tolerance at fixed RON and S.
- Find Co-Optimized fuel blends and engine parameters that maximize speed-load range for acceptable operation of the high-efficiency ACI mode, based on the platform at SNL (Dec).

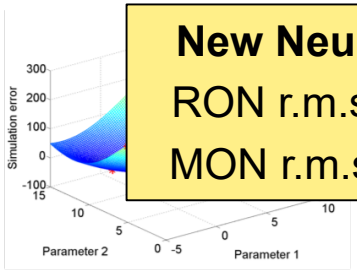
LBNL
- Create multi-level optimization tools for engine models to move beyond static control and allow for a more informative comparison of fuel-engine combinations.
- Extend co-optimizer capabilities to easily handle expensive black-box constraints.
- Use computational optimization tools in co-optimizer to identify fuel properties that are relevant to operational ranges of part-load combustion mode.
- Use computational optimization tools in co-optimizer to explore blendstock feasibility using ANL CFD simulations and to tune simulation model parameters in validation task (model calibration/validation).

**Any proposed future work is subject to change based on funding levels.*

We accelerated hypothesis testing using broad fuel blend explorations for multi-mode operation and BOB optimization





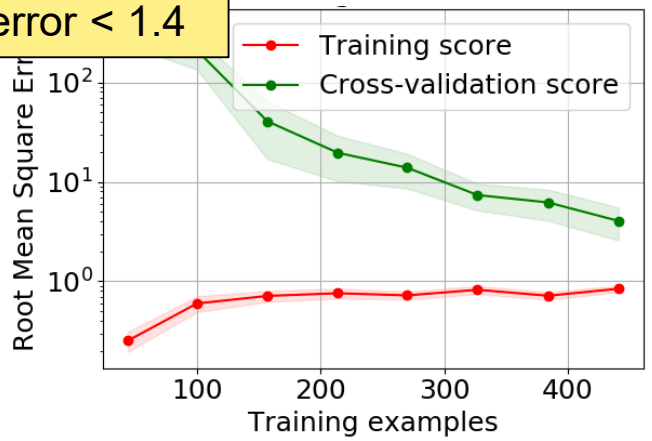


New Neural Network

RON r.m.s. error < 0.8

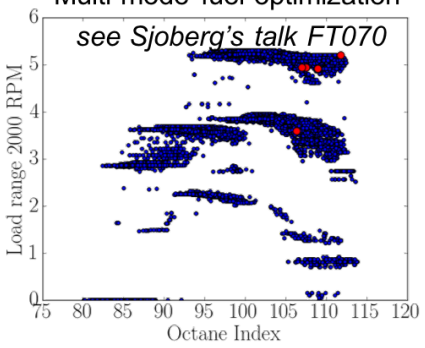
MON r.m.s. error < 1.4

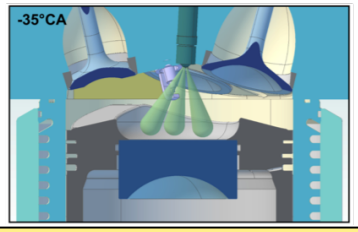
RON Model Training

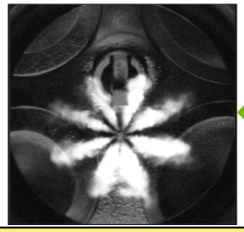


Multi-mode fuel optimization

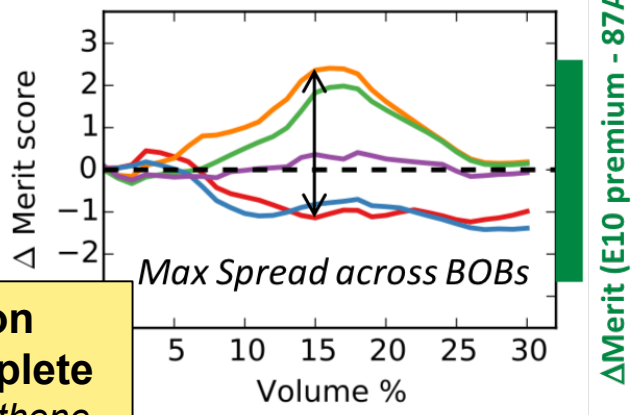
see Sjoberg's talk FT070







Ethanol



Accelerated kinetics-based multi-mode engine simulation

- Over 50,000 blends simulated
- Model shows octane rating is not sufficient to predict load range or robustness of high-efficiency mode.
- Central Fuel Hypothesis fails?

BOB Optimization
Phase 2 - 60% complete
(Max Olefin, Max Naphthene and Max Aromatic tested)